Electronic Supplementary Material (ESI) for CrystEngComm.
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Supplementary Information

Growth mechanism of AlN on hexagonal BN/sapphire substrate by metal-organic chemical vapor deposition

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I. AFM images of hBN and hBN-O_2 layers on sapphire

Fig. S1 shows the AFM images of hBN layer on sapphire with/without O_2 plasma treatment (hBN-O_2/hBN). The wrinkles (the bright wires) and multilayer islands (the bright regions) are clear on the surface of hBN layer, which is consistent with the SEM image. Meanwhile, the AFM image of hBN-O_2 layer is consistent with the SEM image for the decrease of wrinkles.

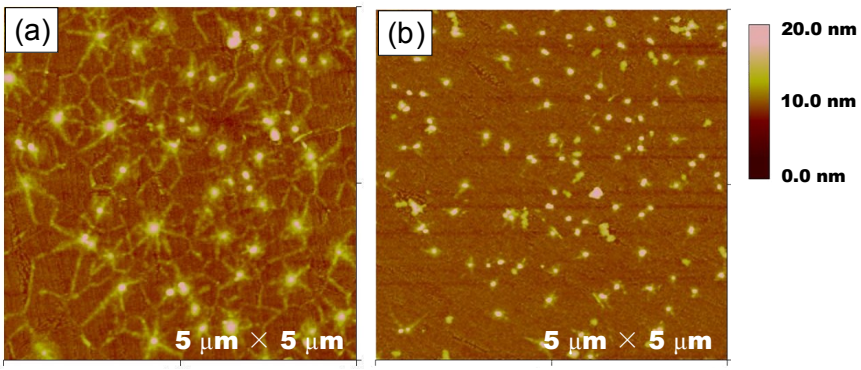

Fig. S1 AFM images of hBN and hBN-O_2 on sapphire

II. Experiment results of 1.45-μm AlN grown on sapphire

Fig. S2 shows the results of AlN directly grown on sapphire. Fig. S2(a) presents the AlN on sapphire has a smooth and flat surface, and the RMS roughness in the 5×5 μm^2 area is only 0.22 nm. Fig. S2(b) and Fig. S2(c) show the ω-scan (rocking curve) profiles of (0002) and (10-12) AlN, respectively. As estimated from the XRD FWHM, the densities of screw and edge dislocations are 1.55×10^8 cm^{-2} and 9.53×10^9 cm^{-2}, respectively.

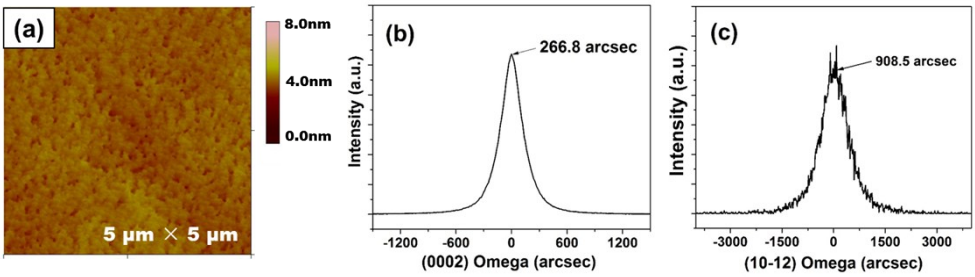

Fig. S2 Experimental results of AlN on sapphire: (a) AFM image, X-ray rocking curves of (b) (0002) and (c) (10-12) AlN grown on sapphire (the number is FWHM value)

III. AFM images of 2-min LT-AlN

Fig. S3 shows the AFM images of the LT-AlN films grown for 2 min on hBN/sapphire, hBN-O_2/sapphire and sapphire. Some hBN multilayer islands can be observed on hBN/sapphire and hBN-O_2/sapphire. At the same time, AlN on hBN-O_2 presents the different morphology comparing with the hBN-O_2 layer before the growth of LT-AlN while the surface of AlN on hBN is nearly the same as the hBN layer before the growth. The uniform AlN islands even cover all the surface of hBN-O_2/sapphire on these regions without hBN multilayer islands, corresponding with the morphology of AlN islands on sapphire. These AFM results are consistent with the SEM results.

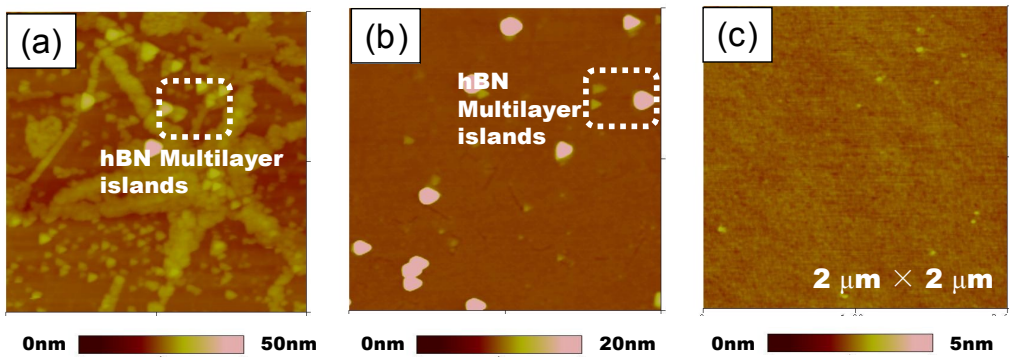

Fig. S3 AFM images of LT-AlN grown for 2 min on hBN/sapphire, hBN-O_2/sapphire and sapphire

IV. Crystal orientation of the AlN films on hBN/sapphire and hBN-O_2/sapphire

Fig. S4 shows the XRD pole figures of {10-12} reflections (2θ =49.9°) of AlN located at ψ= 42° and {11-23} reflections (2θ =43.4°) of sapphire located at ψ= 60° and ψ= 63° with the hBN and hBN-O_2 release layers. It's obviously that AlN on the two substrates shows a clear six-fold rotational symmetry from the {10-12} poles of AlN films indicating the consistent in-plane crystal orientation of AlN domains. Moreover, the ϕ values with the maximum reflection intensity of {10-12} reflections of AlN are approximately equal to the ϕ values with the maximum reflection intensity of {11-23} reflections of sapphire (The measurement accuracy of the XRD pole figure used in our work is 3°.), as shown in table S1. So the two AlN epitaxial layers are both crystallographically rotated by 30° with the structures of (0001)[10-10]AlN||(0001)[11-20]sapphire.

Table S1 the ϕ values of AlN {10-12} pole and sapphire {11-23} poles

release layer	reflection	ψ (°)	φ (°)					
hBN	AlN {10-12}	42	4.5	64.5	121.5	181.5	244.5	304.5
	sapphire {11-23}	60	4.5	61.5	121.5	181.5	244.5	304.5
hBN-O_2	AlN {10-12}	42	1.5	61.5	118.5	178.5	241.5	301.5
	sapphire {11-23}	63	4.5	64.5	121.5	181.5	244.5	304.5

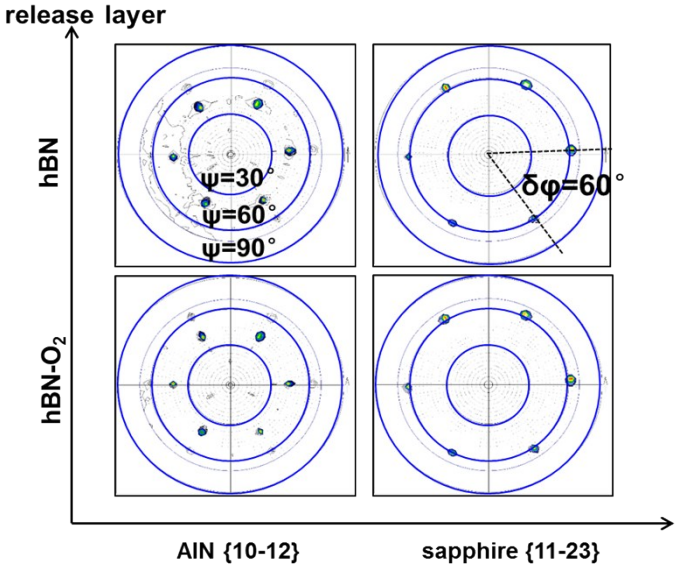

Fig. S4 XRD pole figures of AlN {10-12} reflections and sapphire {11-23} reflections on hBN/sapphire and hBN-O_2/sapphire

V. The transfer process of hBN layer by the aid of PMMA

i) The thin film layer of 4.5% PMMA diluted in anisole was spin coated onto the better hBN side of the Cu foil to support and protect hBN layer.

ii) The PMMA/hBN/Cu sample was baked at about 110 °C for 15 min and then cooled to room temperature.

iii) The hBN on the backside of the Cu foil was washed away by DI water after etching in 10% ferric trichloride solution for 10 seconds.

iv) The Cu substrate continued to be set in the solution for several hours until the etching procedure was done.

v) DI water washed the sample to remove contamination from the solution.

vi) The hBN/PMMA films were transferred onto *c*-plane sapphire substrate and dried in the air.

vii)The sample was baked at 110 °C for 1 hour to reduce numerous wrinkles in the hBN layer.

viii) PMMA was removed by acetone. Finally, the sample was annealed at around 550 °C under a H_2 atmosphere for 30 min to eliminate the PMMA residues and the transfer of the hBN was accomplished.